

Chemistry & Materials Science Directorate
2003



Lawrence Livermore National Laboratory
UCRL-AR-129465-03



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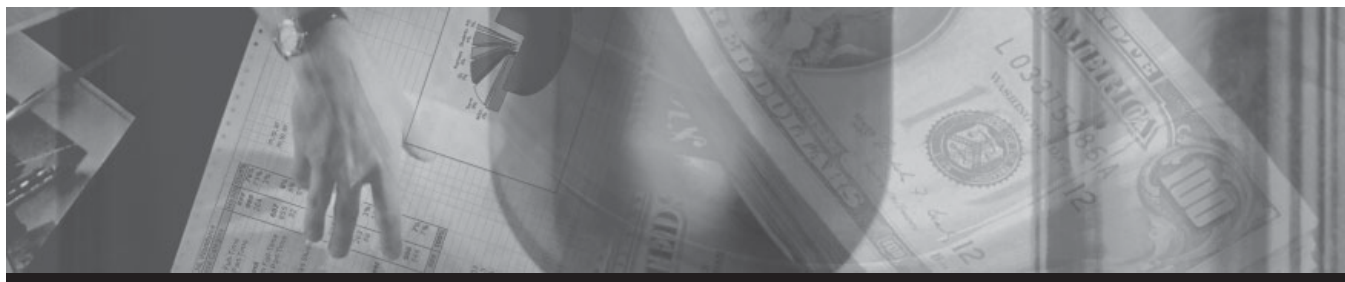
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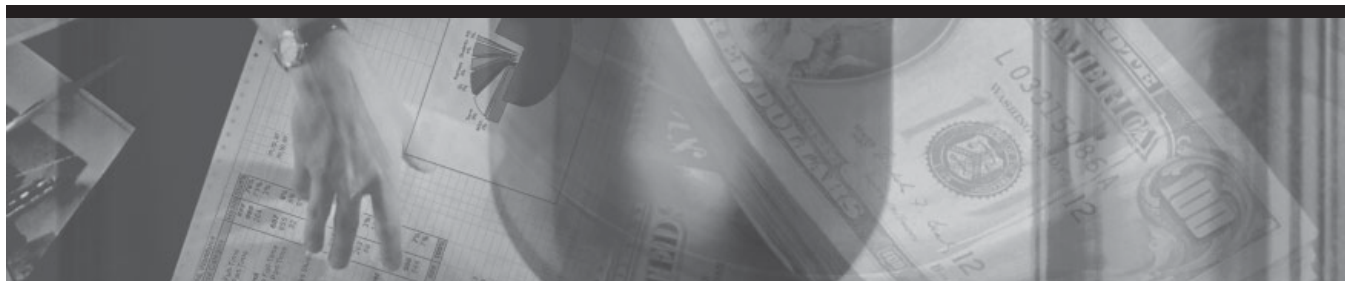
...and a general
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FACTS & FIGURES

Chemistry & Materials Science Directorate
2003

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Acronyms and Abbreviations

Acronyms

AA	associate in arts	ES&H	environment, safety, and health
AD	Associate Director		
AHRD	Administration and Human Resources Directorate	EWSF	Explosives Waste Storage Facility
ANCD	Analytical and Nuclear Chemistry Division	EWTF	Explosives Waste Treatment Facility
BBRP	Biology and Biotechnology Research Program	FSC	Forensic Science Center
BS	bachelor of science	FTE	full-time equivalent
BSNL	BioSecurity and Nanosciences Laboratory	FY	fiscal year
CAFÉ	Cost Accounts Funding Effort	G&A	general and administrative
CAS	Classified Administrative Specialist	GTSI	Glenn T. Seaborg Institute
CChED	Chemistry and Chemical Engineering Division	HC	hazards control
CES	Chemistry & Materials Science Environmental Services	HE	high explosives
CMS	Chemistry & Materials Science	HWM	hazardous waste management
CSP	Computer Security Program	ICF	inertial confinement fusion
DDL	Deputy Division Leader	IGPE	institutional general-purpose equipment
DL	Division Leader	ISMS	Integrated Safety Management System
DMS	Division of Materials Sciences	LDRD	Laboratory Directed Research and Development
DNT	Defense and Nuclear Technologies	LITE	Laboratory institutional time entry
DoD	Department of Defense	LLNL	Lawrence Livermore National Laboratory
DOE	Department of Energy	LS&T	Laser Science & Technology
E&E	Energy & Environment	LTRAIN	Laboratory Training Records and Information Network
EE	electronic engineering		
EMC	Energetic Materials Center	LW	Laboratory-Wide Competition
ERD	Exploratory Research in the Disciplines	ME	mechanical engineering
		MPL	Materials Program Leader

MS	master of science	PhD	doctor of philosophy
MSTD	Materials Science and Technology Division	PMC	program management charge
NAI	Nonproliferation, Arms Control, and International Security	QA	quality assurance
NIF	National Ignition Facility	R&D	research and development
NNSA	National Nuclear Security Administration	S&T	science and technology
OBES	Office of Basic Energy Sciences	SCL	Scientific Capability Leader
OFC	organizational facility charge	SEGRF	Student Employee Graduate Research Fellowship
OJT	on-the-job training	SI	Strategic Initiative
OPC	organizational personnel charge	SSEP	Safety, Security, and Environmental Protection
PARD	protect as restricted data	TBD	to be determined
PAT	Physics and Advanced Technologies	UC	University of California
PEL	Program Element Leader	USI	Undergraduate Summer Institute
		YMP	Yucca Mountain Project

Abbreviations

\$K	thousands of dollars	Ge	germanium
\$M	millions of dollars	gen.	general
admin.	administrative	info.	information
B132N	Building 132 North	lab.	laboratory
B133	Building 133	Lab. Serv.	Laboratory Services
B151	Building 151	ldr.	leader
B154	Building 154	mgmt.	management
B235	Building 235	mgr.	manager
B241	Building 241	ops.	operations
chem.	chemical	prog.	program
Comp.	Computation	Pu	plutonium
coord.	coordinator	rad.	radiological
dep.	deputy	radchem.	radiochemistry
dept.	department	rep.	representative
div.	division	S200	Site 200 (Lawrence Livermore main site)
Eng.	Engineering	S300	Site 300 (Lawrence Livermore explosives testing site)
fab.	fabrication		
Ga	gallium	sec.	secretary



Message from Tomas Diaz de la Rubia

This is the first issue of *Facts & Figures* since my appointment as the Associate Director (AD) for Chemistry & Materials Science (CMS). I welcome new readers and ask for thoughts from both first- and long-time readers regarding this publication.

Facts & Figures has evolved over the years to keep pace with the growth of CMS. The title of this publication reflects its origins and intent—to be a broad overview of budgetary, personnel, and other administrative information about Lawrence Livermore National Laboratory (LLNL) and our Directorate.

The Laboratory is 51 years old, and since its inception, Chemistry, as a discipline, has been identified as a separate organization. I am proud to be a part of a dynamic team and look forward to a very exciting, but challenging, 2003. It is our tradition of excellence in meeting the demands of the Laboratory and in anticipating its future needs through innovations in science and technology that positions us to be an essential part of anticipating and meeting the challenges and opportunities of the future. We are poised for collective success.

Cheers,
Tomas

2002 AT A GLANCE

THE LABORATORY

7,081 career employees, 874 term appointments, 142 postdoctoral researchers, 796 non-career employees, and 745 other non-LLNL laborers.

Laboratory Organization

Director; Deputy Director Science and Technology; Laboratory Executive Officer; Deputy Director Operations; Defense and Nuclear Technologies (DNT); National Ignition Facility (NIF) Programs; Nonproliferation, Arms Control, and International Security (NAI); Energy & Environment (E&E); Physics and Advanced Technologies (PAT); Biology and Biotechnology Research Program (BBRP); CMS; Engineering; Computation; Safety, Security, and Environmental Protection (SSEP); Administration and Human Resources Directorate (AHRD); Laboratory Services

Laboratory Operating Costs

\$1,230M

Laboratory Full-Time Equivalents

7,457

CHEMISTRY & MATERIALS SCIENCE

360 career employees, 62 term appointments, 38 postdoctoral researchers, 58 non-career employees, and 13 other non-LLNL laborers

CMS Organization

AD; Principal Deputy AD; Deputy AD for Science and Technology; Deputy AD for Planning, Development, and Personnel; Assurance Manager; Operations Managers; Material Program Leaders for DNT, NIF, E&E, NAI, and the Department of Defense Technologies; Analytical and Nuclear Chemistry Division; Chemistry and Chemical Engineering Division; Materials Science and Technology Division; Glenn T. Seaborg Institute; BioSecurity and Nanoscience Laboratory; Materials Research Institute

CMS Operating Costs

\$48.1M

CMS Full-Time Equivalents

401



Facts & Figures—Lawrence Livermore National Laboratory

History

The single event that triggered the establishment of Lawrence Livermore National Laboratory was the detonation of the first Russian atomic bomb in 1949. Some American scientists were alarmed that the Soviets could advance quickly to the next step, the hydrogen bomb, with potential disaster for the West. Ernest Lawrence was a key participant in the World War II atomic bomb project at Los Alamos, a Nobel laureate, and founder of the University of California (UC) Radiation Laboratory at Berkeley. Edward Teller was a brilliant physicist at the Los Alamos nuclear weapons laboratory. They met in October of 1949 to discuss the Russian threat.

It was essential, Teller came to believe in the course of the next several years, to start a second nuclear weapons laboratory—to provide competition, to diversify expertise, and to handle the large volume of work that future fast-breaking discoveries would bring. Lawrence supported Teller's proposal for a second weapons lab, and he wanted it established at Livermore. Moreover, he wanted Teller to oversee setting up the new lab.

Teller presented his case to Atomic Energy Commission Chairman Gordon Dean on April 4, 1951, in Washington, D.C. In July 1952, formal Atomic Energy Commission action created the Livermore branch of the UC Radiation Laboratory. In September, this second weapons laboratory opened its doors at the site of a former naval air station, in the sleepy cow town of Livermore, California. Among the group of young Berkeley scientists who were working with Lawrence was 32-year-old Herbert F. York. Barely three years out of graduate school, York was singled out by Lawrence to head the new laboratory.

York set out to develop the Laboratory's program and created four main elements: Project Sherwood (the Magnetic Fusion Program), diagnostic weapon experiments (both for Los Alamos and Lawrence

Livermore), the design of thermonuclear weapons, and a basic physics program. The first two facilities were a building to house the latest electronic computer, a Univac, and a technology building with a large central bay for lifting heavy equipment.

In the early days, Lawrence Livermore's focus was on national needs and technical opportunities. Experts in chemistry, physics, and engineering had a common understanding of the Laboratory's mission and developed new technologies on their own. But along with this went a team effort to understand problems and to work them out together.

Over the following five decades, this new facility was destined to be a competitor of Los Alamos in the development of U.S. nuclear deterrents. Lawrence Livermore was also to become one of the world's premier scientific centers, using its knowledge of nuclear science and engineering to break new ground in energy, computations, biomedicine, and environmental science.

Mission

Lawrence Livermore is a premier applied-science, national-security laboratory. Its primary mission is to ensure that the nation's nuclear weapons remain safe, secure, and reliable and to prevent the spread and use of nuclear weapons worldwide.

This mission enables Laboratory programs in advanced defense technologies, energy, environment, biosciences, and basic science to apply Livermore's unique capabilities and to enhance the competencies needed for the national-security mission.

The Laboratory serves as a resource to the U.S. government and as a partner with industry and academia.

Vision and Goals

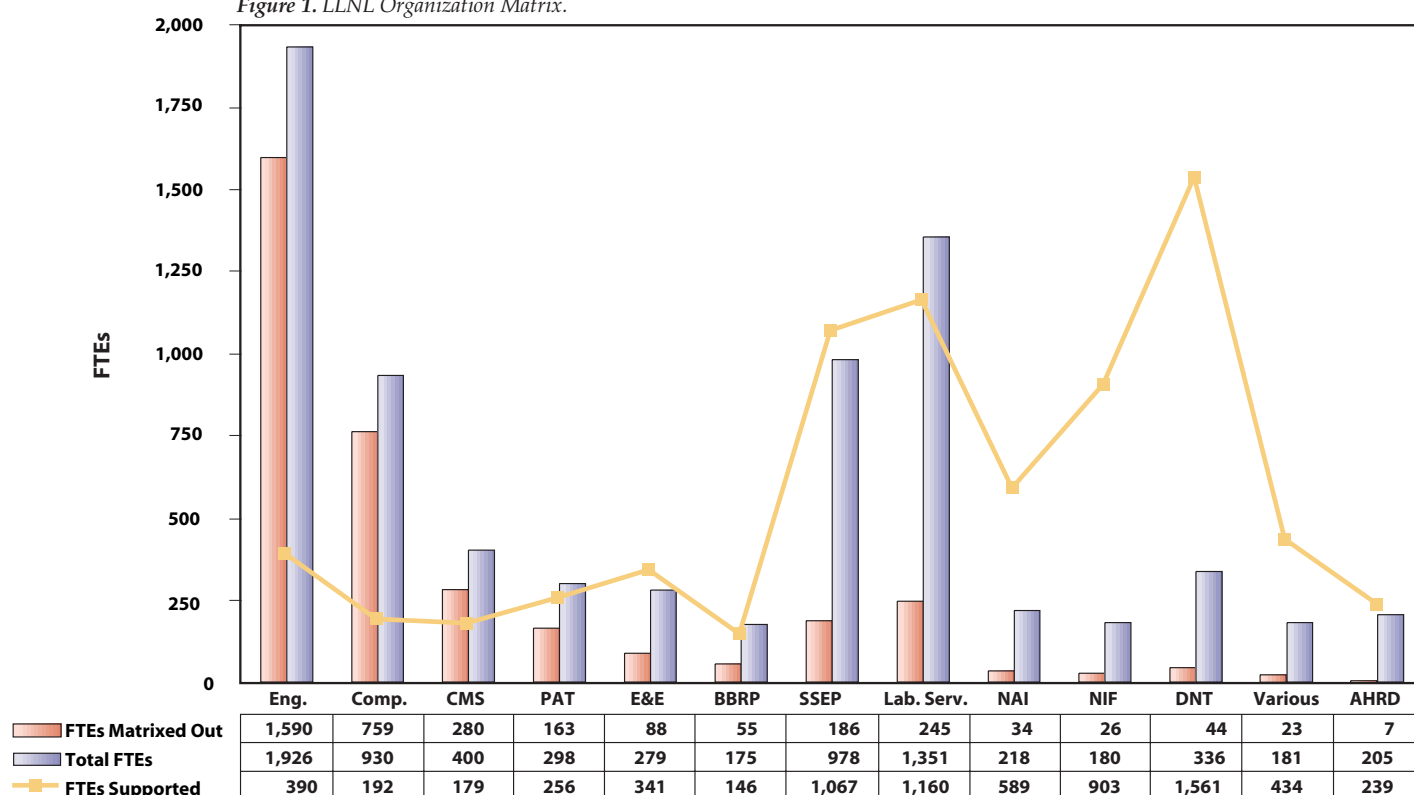
The Laboratory's goal is to apply the best science and technology (S&T) to enhance the security and well-being of the nation and to make the world a safer place.

Operations

Laboratory programs are supported by a large technical base consisting of more than 1,000 PhD scientists and engineers. A significant portion of the scientific staff is organized into “disciplines” or support directorates—CMS, Computation, and Engineering, and many of these people are matrixed, or assigned, to specific programs within other directorates. Use of the matrix system fosters the efficient transfer of technical knowledge among programs,

enables staff members to develop a wide-ranging set of skills and knowledge, and infuses projects with diverse ideas for solutions. As a result, the Laboratory has the ability to seize program opportunities, the agility to react quickly to technical surprises, and the flexibility to respond to programmatic changes. Figure 1 shows the percentages of Laboratory employees matrixed out to different directorates, along with the total number of FTEs and the mix of FTEs supported by each organization.

Figure 1. LLNL Organization Matrix.



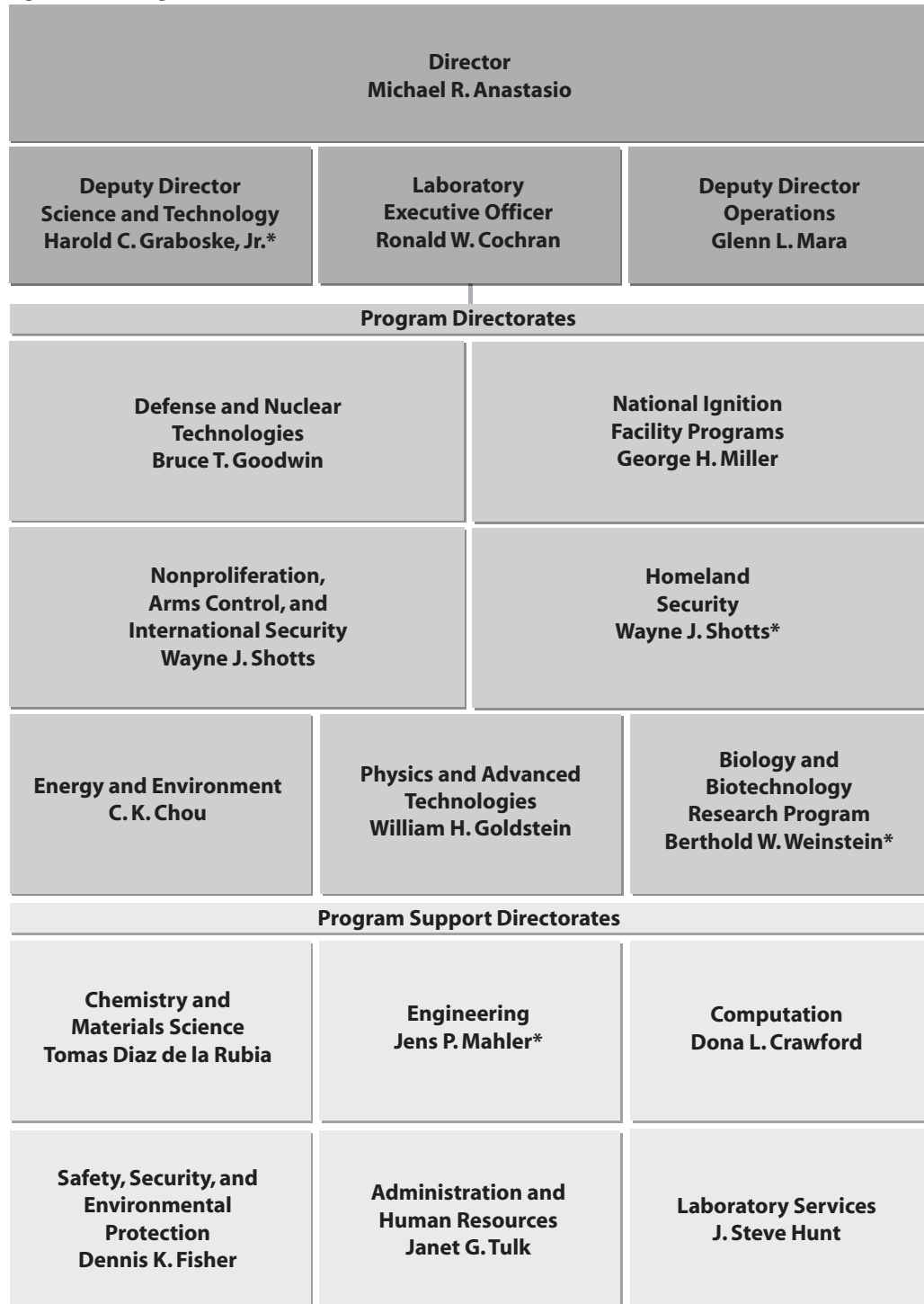
	% Matrixed Out	Eng.	Comp.	CMS	PAT	E&E	BBRP	SSEP	Lab. Serv.	NAI	NIF	DNT	Various	AHRD	FTEs Supported	FTEs Matrixed In
Eng.	83	336	24	4	2	1	2	11	10	—	—	—	—	1	390	55
Comp.	82	9	171	—	—	—	—	1	9	—	—	—	—	—	192	21
CMS	70	16	17	120	2	1	1	19	2	—	1	—	—	—	179	59
PAT	55	78	19	5	135	—	1	6	4	—	4	3	1	—	256	121
E&E	31	46	51	29	1	192	3	10	9	—	—	—	—	—	341	149
BBRP	31	2	16	—	—	1	121	3	2	—	—	—	—	1	146	25
SSEP	19	83	104	13	1	8	—	792	52	—	1	11	1	2	1,067	275
Lab. Serv.	18	6	18	2	—	—	—	27	1,106	—	—	—	—	—	1,160	54
NAI	15	145	105	39	14	33	29	19	13	184	—	8	—	—	589	405
NIF	15	515	83	45	15	—	—	21	56	1	154	13	—	—	903	749
DNT	13	623	291	122	100	21	—	55	37	17	2	292	—	1	1,561	1,269
Various	13	58	24	22	26	20	19	12	37	14	15	9	177	2	434	276
AHRD	3	8	8	—	3	3	—	1	14	1	2	—	1	198	239	41
Total FTEs		1,926	930	400	298	279	175	978	1,351	218	180	336	181	205	7,457	3,499

Minor variances may occur due to rounding.
Dated: September 30, 2002

Organization

No standardized organizational structure exists within the program and support directorates. Each directorate is organized by its AD to efficiently meet the needs and mission of the Laboratory (see Figure 2).

Figure 2. LLNL Organization Chart.



*Acting

Financial and Full-Time-Equivalent Highlights

For the fiscal year (FY) ending on September 30, 2002, the operating and capital expenses totaled \$1,542.9M. This included \$1,229.5M for Laboratory operating budgets and \$313.3M for capital projects. FY03 operating and capital budgets are projected to be \$1,595.3M. The staffing level as of September 30, 2002, was 7,457 full-time equivalents (FTEs), including full-time, part-time, and indeterminate-time employees. As of December 28, 2002, there are 7,828 planned FTEs. (See Table 1 for the breakdown of financial and FTE information by major program.) FTE is a term used to describe a full-time employee who, during the course of a year, takes an average amount of vacation, sick leave, and other leave in addition to normal holiday leave. Part-time employees are counted as fractional FTEs. Therefore, FTE totals are not equivalent to the number of employees.

Figures 3 and 4 show the operating costs and FTEs from FY93 to FY02.

Figure 3. Laboratory Operating Costs during the Past 10 Years.

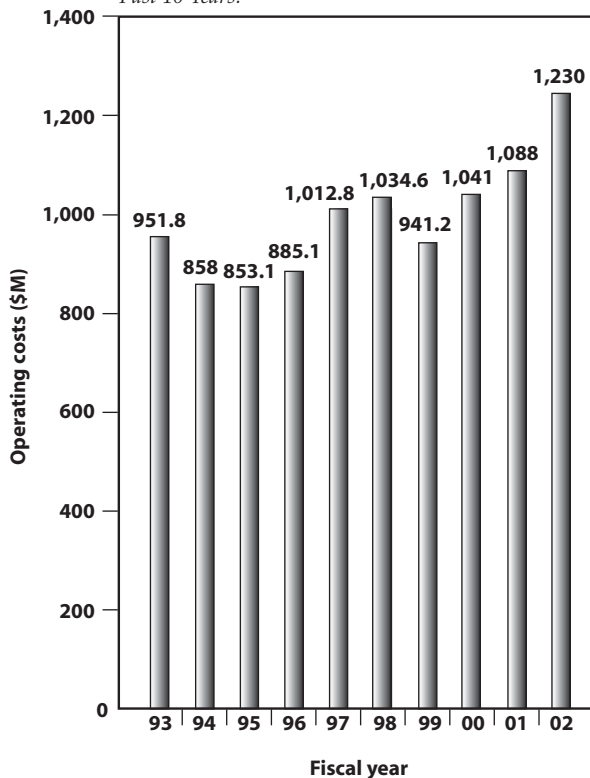
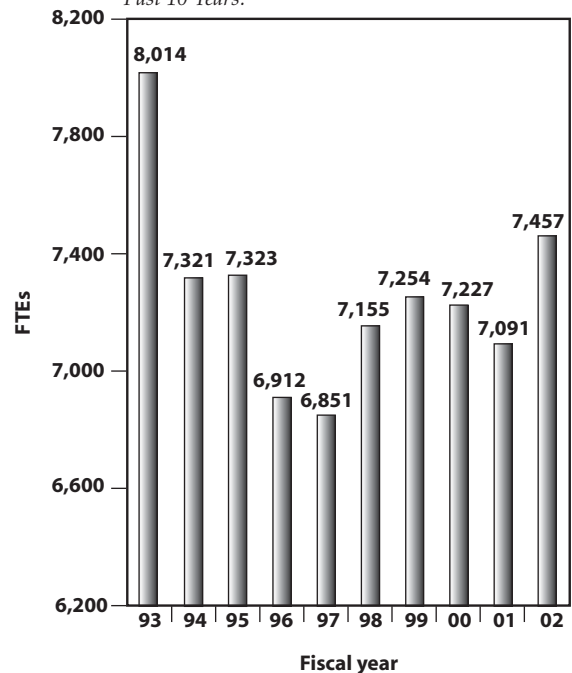


Figure 4. Number of Laboratory FTEs during the Past 10 Years.*



*Does not include postdoctoral researchers or retirees

Table 1. Laboratory Costs (\$M) and FTEs by Major Program.

Major Program	FY02 Actual 9/30/02		FY03 Planned as of 12/28/02	
	\$M	FTEs	\$M	FTEs
Operating Costs				
Stockpile Stewardship & Management	435.5	1,216.4	445.4	1,245.6
Advanced Simulation and Computing Platforms & Alliances	52.5	—	63.0	—
Facilities and Infrastructure	6.4	0.5	6.0	0.4
Safeguards & Security	90.3	485.9	79.3	511.2
Inertial Confinement Fusion	39.1	99.6	43.4	108.8
National Ignition Facility (NIF)	90.7	246.5	93.7	344.0
Nonproliferation	117.7	219.5	141.7	261.1
Other National Nuclear Security Administration (NNSA)	1.5	0.1	1.6	0.1
Intelligence	8.2	26.2	8.8	28.2
Environmental Restoration & Waste Management	42.1	163.4	52.8	177.2
Fusion Energy	14.6	46.3	15.9	46.8
Biomedical & Environmental Research	24.6	107.8	27.7	106.6
Office of Basic Energy Sciences	14.1	31.4	15.5	34.2
Energy Research	10.4	30.0	12.3	32.1
Other Department of Energy (DOE)	17.1	48.9	13.3	52.2
Work for DOE	121.1	270.4	89.5	239.1
Non-DOE	143.5	357.6	171.3	363.4
Total Sponsor-Funded Operating Costs	1,229.5	3,350.5	1,281.1	3,551.0
Capital Costs				
NIF Capital Construction	277.2	404.8	210.0	380.2
NNSA Construction	27.6	4.0	63.9	1.2
NNSA General Plant Project	5.9	0.5	37.4	1.6
DOE Line Item Construction	2.7	—	3.0	9.0
Total Sponsor-Funded Capital Costs	313.3	409.3	314.2	392.0
Total Sponsor-Funded Operating & Capital Costs	1,542.9	3,759.8	1,595.3	3,943.0
Distributed Costs				
Laboratory Directed Research & Development	—	269.7	—	273.9
Plant Engineering Jobs	—	535.1	—	559.5
Organizational Facility Charge	—	287.6	—	307.2
Organizational Personnel Charge	—	587.3	—	617.4
Program Management Charge	—	367.6	—	396.6
Distributed Service Center	—	397.4	—	430.5
Institutional General-Purpose Equipment	—	9.1	—	5.6
General & Administrative	—	1,243.2	—	1,294.1
Total Distributed Costs	—	3,697.0	—	3,884.8
Total Operating, Capital, & Distributed Costs	1,542.9	7,456.8	1,595.3	7,827.8
Minor variances may occur due to rounding.				

Staffing and Demographics

As of September 30, 2002, the LLNL workforce (by head count) numbered 9,638. This workforce is composed of 73% career employees, 9% term appointments, 1% postdoctoral researchers, 8% non-career employees (including temporary, student, faculty, retiree, and miscellaneous employees), and 8% supplemental laborers (see Table 2). According to the staff profile of indefinite employees, 39% are scientific staff, 22% are administrative and clerical personnel, and 39% are technical and crafts personnel. About 45% of the scientists and engineers have PhDs. For a listing of staff by degree composition and job title, see Table 3. The technical discipline makes up the largest job group (27%). LLNL's scientific staff is shown by discipline, along with the number of postdoctoral researchers, in Table 4.

Table 2. LLNL Workforce.

Workforce Category	FY93	FY94	FY95	FY96	FY97	FY98	FY99	FY00	FY01	FY02
Career employees	7,850	7,079	6,994	6,583	6,367	6,567	6,668	6,488	6,613	7,081
Term appointments	135	202	489	561	597	708	808	788	687	874
Postdoctoral researchers	153	168	168	134	109	122	144	104	103	142
Non-career employees	840	925	642	555	566	616	608	565	687	796
Other laborers (non-LLNL)	1,510	1,222	912	627	810	806	664	559	567	745
Total Laboratory Heads	10,488	9,596	9,205	8,460	8,449	8,819	8,892	8,504	8,657	9,638

10-Year LLNL Population Distribution by Workforce Category

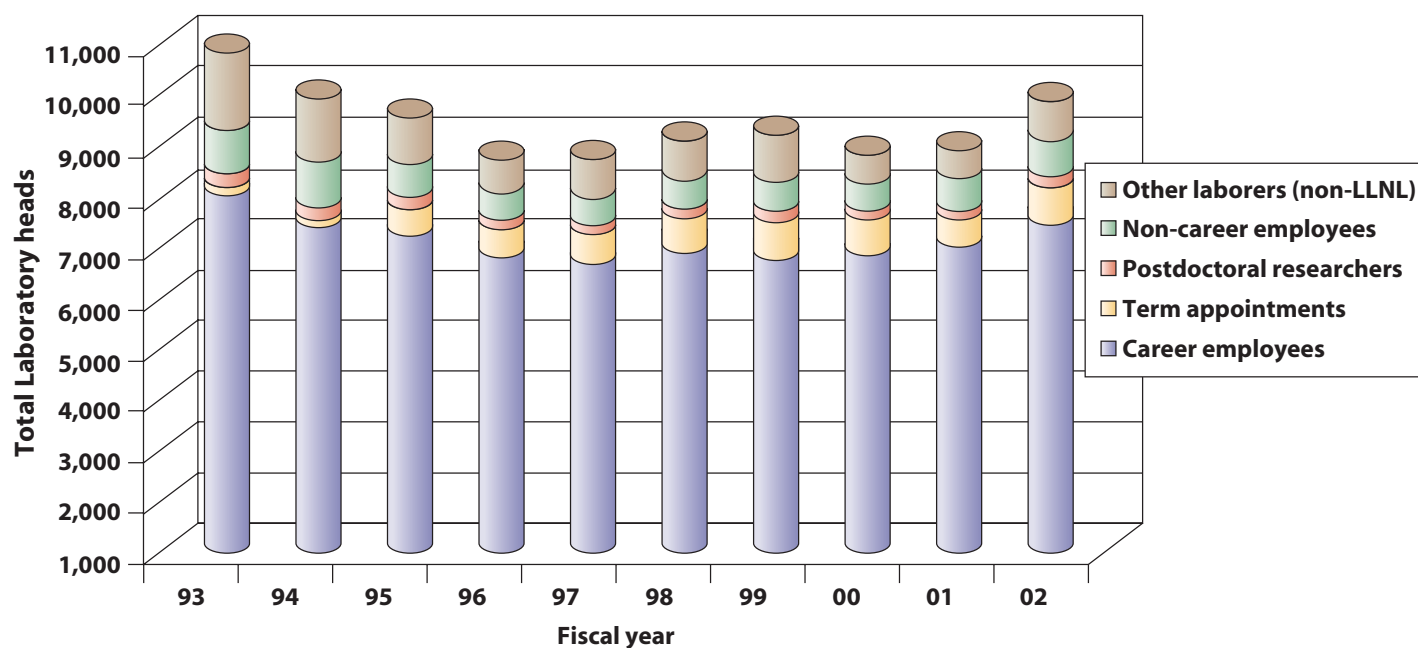


Table 3. LLNL Staff Profile by Job Title and Degree Composition.

Job Title	PhD	MS	BS	AA	No degree	Total	Staff (%)
Scientists & Engineers	1,253	794	708	9	41	2,805	39
Physicist—(270)	666	82	27	—	2	777	11
Chemist—(242)	136	38	44	—	1	219	3
Engineer/Patent Engineer—(168, 249)	268	392	279	2	16	957	13
Mathematician/Computer Scientist—(256, 285)	100	217	301	5	22	645	9
Biological Scientist—(225, 277, 235, 228, 221)	21	16	19	1	—	57	1
Environmental Scientist—(230)	15	35	33	—	—	83	1
Metallurgist—(265)	34	7	2	1	—	44	1
Medical Doctor (Staff)—(263)	4	—	—	—	—	4	—
Political Scientist—(295)	8	7	3	—	—	18	—
Postdoctoral Research Staff—(220)	1	—	—	—	—	1	—
Administrative & Clerical Personnel	32	161	366	145	883	1,587	22
Management—(196, 197)	20	58	43	4	16	141	2
Professional—(163–165, 169, 170)	4	22	38	1	5	70	1
Administrative—(100–162)	8	79	236	67	323	713	10
Clerical/General Services—(400–462)	—	2	49	73	539	663	9
Technical & Crafts Personnel	2	32	374	722	1,630	2,760	39
Security/Fire Dept.—(051, 055, 650–656)	—	1	30	54	224	309	4
Technical—(302–339, 393, 347–391, 502–588, 593)	2	30	329	607	990	1,958	27
Trades—(722–799, 805–990)	—	1	15	61	410	487	7
Facilities/OJT/Gen. Helper—(700, 701, 704, 801)	—	—	—	—	6	6	—
Total Laboratory Heads	1,287	987	1,448	876	2,554	7,152	100
Degree Composition (%)	18	14	20	12	36	100	
Excludes summer hires and supplemental laborers Minor variances may occur due to rounding. Dated: September 30, 2002							

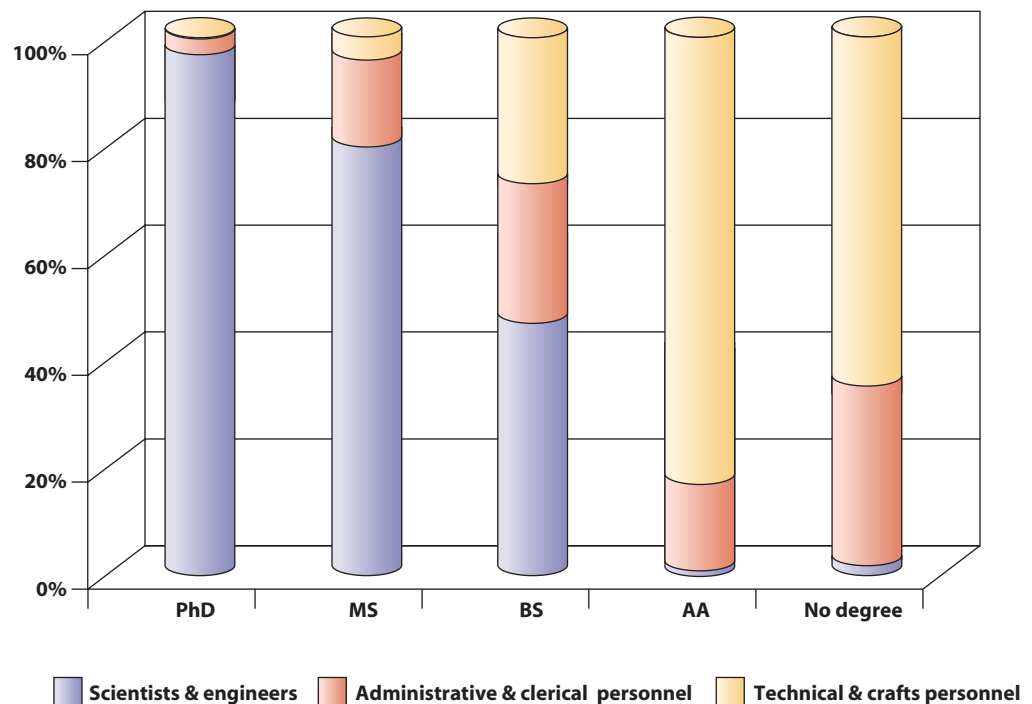
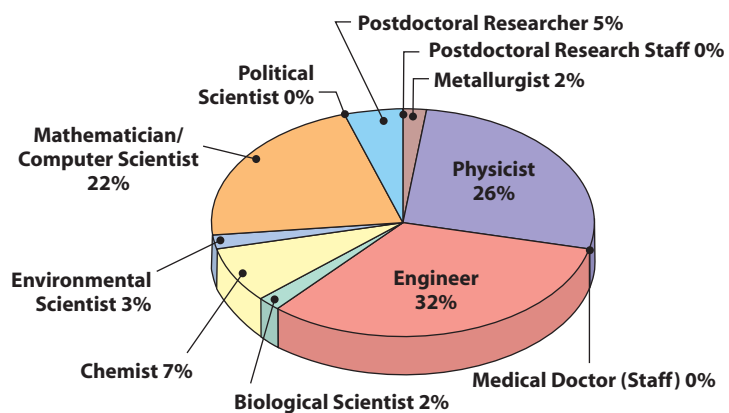


Table 4. LLNL Scientists and Engineers by Discipline and Postdoctoral Researchers.

Job Title	Total	Staff (%)
Scientists & Engineers	2,805	95
Physicist—(270)	777	26
Chemist—(242)	219	7
Engineer/Patent Engineer—(168, 249)	957	32
Mathematician/Computer Scientist—(256, 285)	645	22
Biological Scientist—(225, 277, 235, 228, 221)	57	2
Environmental Scientist—(230)	83	3
Metallurgist—(265)	44	2
Medical Doctor (Staff)—(263)	4	—
Political Scientist—(295)	18	—
Postdoctoral Research Staff—(220)	1	—
Postdoctoral Researchers	142	5
Total Laboratory Heads	2,947	100
Includes indefinite employees and postdoctoral researchers only Minor variances may occur due to rounding. Dated: September 30, 2002		





Facts & Figures—Chemistry & Materials Science

History

Since Lawrence Livermore's inception in 1952, Chemistry, as a discipline, has been identified as a separate organization. It has been called the Chemistry Group; the Chemistry Division; the Chemistry Department; the Chemistry & Materials Science (CMS) Department; and since 1985, the CMS Directorate. Table 5 outlines the major changes in the Chemistry organization since 1952.

Operations

The scientific and technical discipline activities of the CMS Directorate can be divided into three broad categories:

- I. CMS staff assigned to work directly in a program—a matrix assignment typically involving short deadlines and critical time schedules.
- II. The development, management, and delivery of analytical, characterization, measurement, synthesis, processing, and computing capabilities and scientific services to the programs.
- III. Longer-term research-and-development (R&D) activities in technologies important to the programs, determining the focus and direction of technology-based work on programmatic needs.

Integrated Safety Management System

CMS applies Livermore's Integrated Safety Management System (ISMS) to incorporate quality assurance and environment, safety, and health (ES&H) requirements into CMS research and work activities. The focus of CMS ISMS is to provide resources to our scientists and employees to support the accomplishment of research or work activities in ways that fulfill the ES&H requirement to "do work safely."

To achieve the goals of Integrated Safety Management, CMS provides safety officers and ES&H Team 5 as support to our researchers. These resources help researchers complete the Integration Work Sheet process to identify ES&H requirements early in their work planning. This process results in improved project planning and, ultimately, fewer ES&H roadblocks and better budget estimates.

Another strong component of CMS ISMS is our facility safety committees, which operate in each CMS-managed facility at Sites 200 and 300. These committees enable workers to assist in resolving safety issues that affect research and work activities in the Directorate's facilities.

While we continue to seek feedback for continuous improvement, our ISMS has helped us to better define line management's responsibility for work activities and has increased worker involvement in and awareness of safety.

Table 5. Chronological History of CMS Directorate Management from 1952 to the Present.

Year	CMS Directorate Management
1952	The Chemistry Group—50 of the Laboratory's 308 full-time equivalents—reports to E. O. Lawrence through Herb York. Ken Street, Chemistry Department Head
1953	Roger Batzel, Assistant Department Head of Chemistry
1956	Ken Street, Chemistry Division Leader.
1957	Ken Street, Associate Director (AD) of Chemistry.
1959	Ken Street goes to UC Berkeley (he returns to Livermore in 1974 as the Energy Programs AD). The Chemistry Division, under Roger Batzel, reports to Edward Teller.
1961	Roger Batzel, Chemistry AD and acting AD for the Test Directorate (remains Department Head)
1966	Roger Batzel, Chemistry and Space Reactor Program AD
1967	Gus Dorough, Chemistry Department Head
1969	Roger Batzel, Chemistry and Biomedical Research AD
1971	Roger Batzel, LLNL Director James Kane, Chemistry Department Head
1973	Gus Dorough, AD for Scientific Support (which included Chemistry and Computation) The Chemistry Department becomes the Chemistry and Materials Science Department.
1974	James Kane goes to Washington (as Technical Assistant to the General Manager, Atomic Energy Commission; he later became the head of Energy Research. In 1985, Kane was appointed as the Special Assistant for Laboratory Affairs, UC Office of the President, under Senior Vice-President Bill Frazer). Jack Frazer, Chemistry Department Head
1977	The Radiochemistry Division moves to the Nuclear Test Directorate and is renamed the Nuclear Chemistry Division under Chris Gatrousis.
1978	Charles Bender, Chemistry Department Head
1982	Ken Street, Acting AD for Chemistry and Computation
1983	Computation separates from Chemistry, with Bob Borchers as the Computation AD.
1985	Chris Gatrousis, AD for Chemistry & Materials Science (CMS)
1994	Jeff Wadsworth, AD for CMS The Nuclear Chemistry Division rejoins the CMS Directorate.
1996	Larry Newkirk, Acting AD for CMS
1997	Hal Graboske, AD for CMS
2002	Tomas Diaz de la Rubia, AD for CMS

Mission

The mission of the CMS Directorate is to enable the Laboratory to accomplish its primary objectives through excellence in the chemical and materials sciences.

Vision

Our vision is to be seen as the premier provider of scientific leadership that meets and anticipates the needs of the Laboratory, while at the same time being recognized as a national and international leader in the chemical and materials sciences and having an exceptional and safe work environment that attracts and retains a vital and diverse workforce.

Strategic Goals

- Delivering on our commitments and enhancing our intellectual leadership in key areas of the Laboratory
- Excelling in science that ensures program success in responding to national missions
- Performing science and technology of nationally recognized excellence
- Developing and maintaining a high-quality diverse workforce that serves the needs of the Laboratory
- Creating and sustaining a state-of-the-art, cost-effective scientific infrastructure

Organization

In July 2002, Laboratory Director Michael Anastasio announced the selection of Tomas Diaz de la Rubia as the AD for CMS.

Tomas joined the CMS Directorate in 1989 as a postdoctoral researcher, having earned a bachelor of science degree and a PhD in physics in 1984 and 1989 from the State University of New York at Albany.

Prior to becoming the CMS AD, Tomas was the Scientific Capability Leader for Computational Materials Science and the Deputy Division Leader for Science and Technology in CMS's Materials Science and Technology Division. Tomas has also served as the Materials Program Leader for NIF Programs and has led the laser-materials interaction investment area in CMS. In addition, Tomas has played key roles at the Laboratory in the NIF and Stockpile Stewardship Programs, where he participated in developing and applying the multiscale modeling of materials to important programmatic issues.

Tomas has authored and coauthored over 130 publications in the areas of computer simulation of physical properties and the performance of materials. He is an active member of the scientific community and has chaired a large number of national and international conferences and committees. Tomas is a fellow of the American Physical Society and was elected to the board of directors of the Materials Research Society, where he is currently serving a three-year term.

Two Essential Conditions for Success...

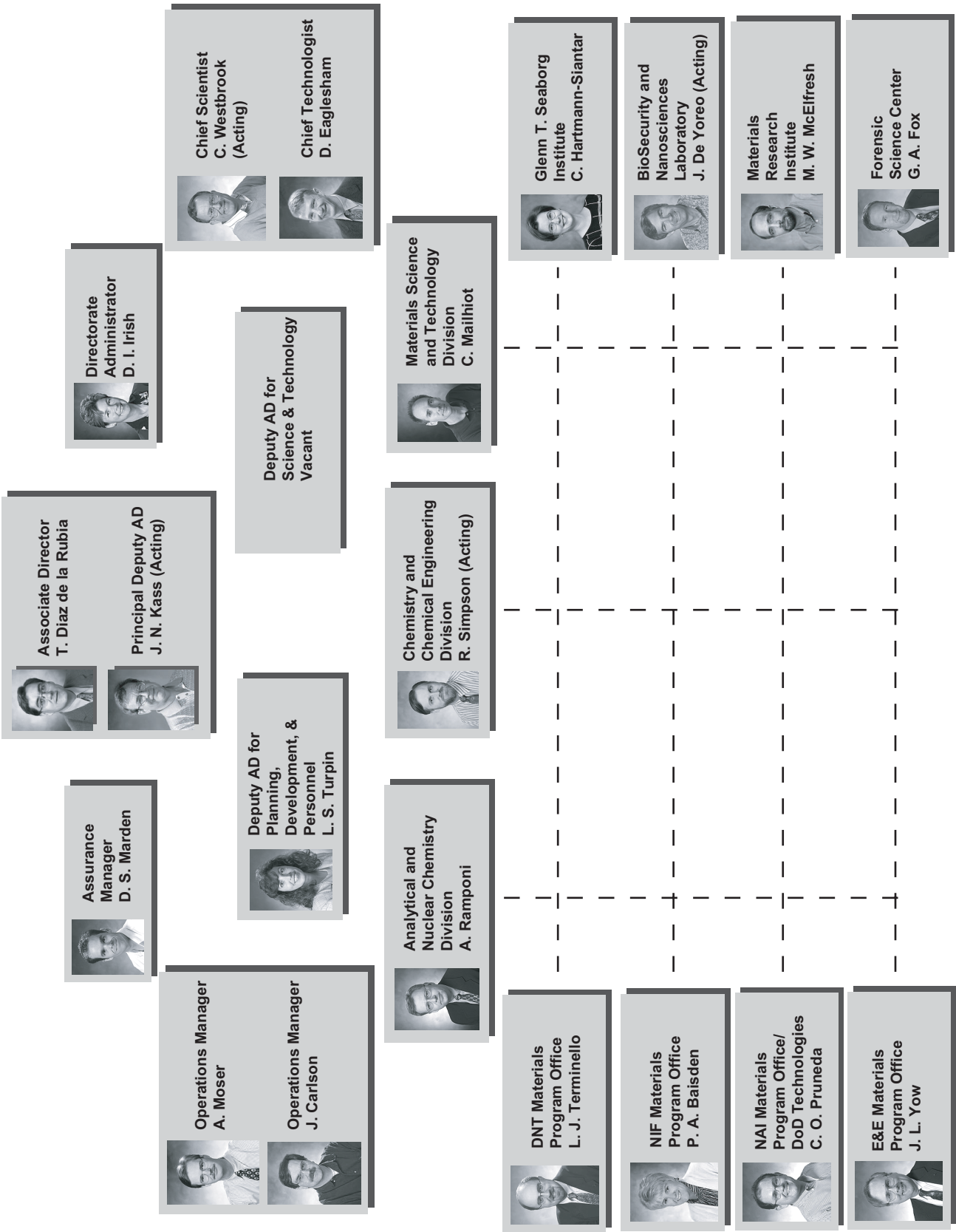
- Deliver on our commitments.
- Anticipate change and capitalize on opportunities through innovations in science and technology.

—Tomas Diaz de la Rubia,
CMS Associate Director

Figure 5 shows the current CMS organization, which includes the leaders of the following:

- Infrastructure activities and functions that span the Directorate:
 - Administration
 - Materials Program Leaders
 - Chief Scientist and Chief Technologist
 - Personnel
 - Assurance oversight
 - Operations
 - Resource management
 - Facility management
 - Security
 - Computer support
- Divisions that support the following overarching themes:
 - Materials properties and performance under extreme conditions—the Materials Science and Technology Division
 - Chemistry under extreme conditions and chemical engineering in support of national-security programs—the Chemistry and Chemical Engineering Division
 - Science in support of national security at the intersection of chemistry, materials science, and biology—the Analytical and Nuclear Chemistry Division
 - Applied nuclear science for human health and national security—the Analytical and Nuclear Chemistry Division
- Institutes and centers that provide strong interdirectorate collaborations, strong connections to the University of California, and a window to the world:
 - Glenn T. Seaborg Institute
 - Materials Research Institute
 - BioSecurity and Nanosciences Laboratory
 - Forensic Science Center

Figure 5. CMS Directorate Organization Chart.



Directorate Awards

Awards under the Directorate Awards and Spot Awards programs recognize one-time achievements that have notable impact on the CMS Directorate and/or that contribute to the pursuit of excellence at Lawrence Livermore. CMS awards are given in the following categories:

- Scientific/technical
- ES&H
- Leadership
- Operations and administration
- Institutional impact

Programmatic contributions are recognized by the program directorates through their awards programs.

Award Types and Criteria

Directorate Quarterly Awards

Directorate Awards are given quarterly, based on the nominations received, and provide individuals or teams with cash awards ranging from \$75 to \$1,000. The criteria for Directorate Awards include the following:

- Significant scientific/technical accomplishment, breakthrough, or discovery
- Outstanding and/or unusual creativity and/or initiative used in accomplishing work assignments, including problem definition and solution
- Significant innovation by an individual or a team that contributes to progress towards the completion of a project milestone
- Exemplary performance to an important organizational need

Table 6 lists the FY02 recipients.

Spot Awards

Spot Awards, which consist of memorabilia and certificates of recognition, are distributed by senior managers. Recipient names are maintained by the division offices. The criteria for Spot Awards include the following:

- Significant improvement of quality, efficiency, safety, and productivity in all categories
- Administrative or management practices that have an organizational effect
- Outstanding achievements in support of CMS Directorate goals or values (e.g., for community service, ES&H, cost-cutting/enhanced efficiency, educational outreach, and diversity)

Table 6. CMS Directorate Quarterly Awards in 2002.

Award Recipient(s)	Accomplishment
Patrick Allen	Materials Research Society symposium organizer, <i>Applications of synchrotron radiation techniques to materials science</i> , April 16–20, 2001
Maria Bartelt	Materials Research Society symposium organizer, <i>Statistical mechanical modeling in materials research</i> , November 25–29, 2001
Ted Baumann, Paul Coronado, Glenn Fox, Alex Gash, Brad Hart, Larry Hrubesh, John Poco, Bob Reibold, John Reynolds, Joe Satcher, Randy Simpson, Tom Tillotson	Applications of ultralow-density materials to multiple LLNL programs, including NAI sensors, DNT energetic composites, DNT/NIF low-density targets, and NIF optics coatings
Sharon Beall, Nancy Schoendienst	Continuing leadership in the development of CAFÉ, including the implementation to other LLNL directorates
Christoph Bostedt	Surface passivation effects of deposited Ge-nanocrystal films probed with synchrotron radiation
Jenean Brothers, Debbie Hackel	Diligence and perseverance in handling and remarking over 450 boxes of the Directorate's PARD
Vasily Bulatov	Materials Research Society symposium organizer, <i>Advances in materials theory and modeling: Bridging over multiple length and time scales</i> , April 16–20, 2001
Geoff Campbell	Materials Research Society symposium organizer, <i>Materials instabilities and patterning in metals</i> , April 17–18, 2001
CMS Information Systems Team	Outstanding service
Virginia Curran	1st recipient of the Darleane Hoffman Graduate Fellowship Award
James De Yoreo	Materials Research Society symposium organizer, <i>Morphology and dynamics of crystal surfaces in molecular and colloid systems</i> , April 16–20, 2001
John Elmer, Todd Palmer, Joe Wong	Work on in situ synchrotron investigations of welds, combined with computer modeling and postweld microstructural characterization
Thomas Felter	Materials Research Society symposium organizer, <i>Advanced materials and devices for large-area electronics</i> , April 17–20, 2002
Patrick Gallagher	Significantly reducing the quantities of legacy chemicals in the CMS Site 300 chemistry area
Eric Gard	Developing a new CMS capability in real-time bioaerosol mass spectrometry and demonstrating that capability for spore detection
Reggie Gaylord	Outstanding support through the timely implementation of gamma-ray spectrometers, analysis, and procedures
Francois Genin	Materials Research Society symposium organizer, <i>Femtosecond materials science technology</i> , April 16–18, 2001
Kurt Glaesemann	2002 Hal Graboske Award for Excellence in Postdoctoral Research in CMS
Sonia Letant	2002 Postdoctoral Program Symposium: Outstanding Poster Presentation
Allen Lingenfelter, Dan McCright	Materials Research Society symposium organizer, <i>Nuclear waste containment materials</i> , April 19, 2001
Christine Orme	Materials Research Society symposium organizer, <i>Biological and biomimetic materials: Properties to function</i> , April 1–5, 2002
Doug Phinney	Outstanding contributions to institutional workforce development and external interactions by organizing the 2002 Nuclear Science Internship Program for the Glenn T. Seaborg Institute
Barbara Pulliam, David Sprayberry	Diligence and dedication to the Trailer 2475 construction and the B-4 parking-lot-upgrade projects
Andrew Quong	Materials Research Society symposium organizer, <i>Fundamental studies of corrosion and oxidation</i> , April 17–19, 2001

Staffing and Demographics

As of September 30, 2002, the CMS workforce (by head count) numbered 531. This workforce is composed of 68% career employees, 12% term appointments, 7% postdoctoral researchers, 11% non-career employees, and 2% supplemental laborers (see Table 7). Table 8 shows a staff profile by degree composition for career employees, with a head count of 369. The staffing breakdown is 70% scientists and engineers, 17% technicians, and 13% administrative and clerical personnel.

Table 7. CMS Workforce.

Workforce Category	FY96	FY97	FY98	FY99	FY00	FY01	FY02
Career employees	303	300	327	338	342	341	360
Term appointments	42	46	55	58	52	51	62
Postdoctoral researchers	24	25	26	31	22	20	38
Non-career employees	34	32	36	34	31	50	58
Other laborers (non-LLNL)	2	2	8	8	9	15	13
Total CMS Heads	405	405	452	469	456	477	531

7-Year CMS Population Distribution by Workforce Category

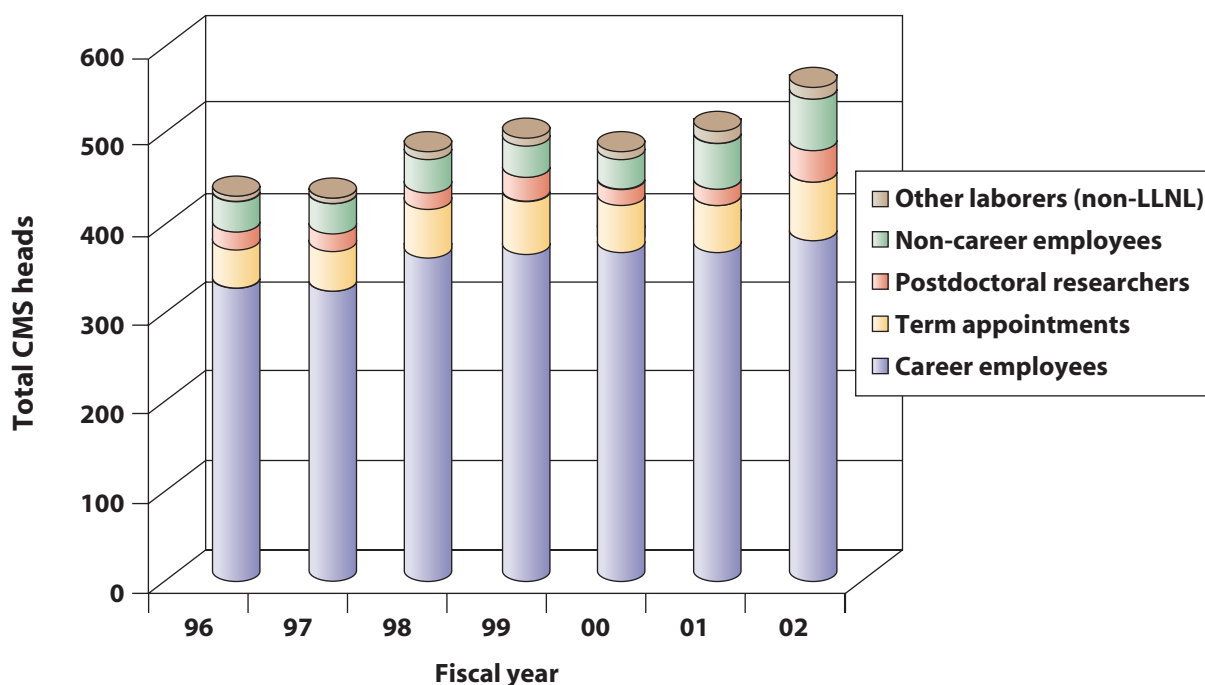
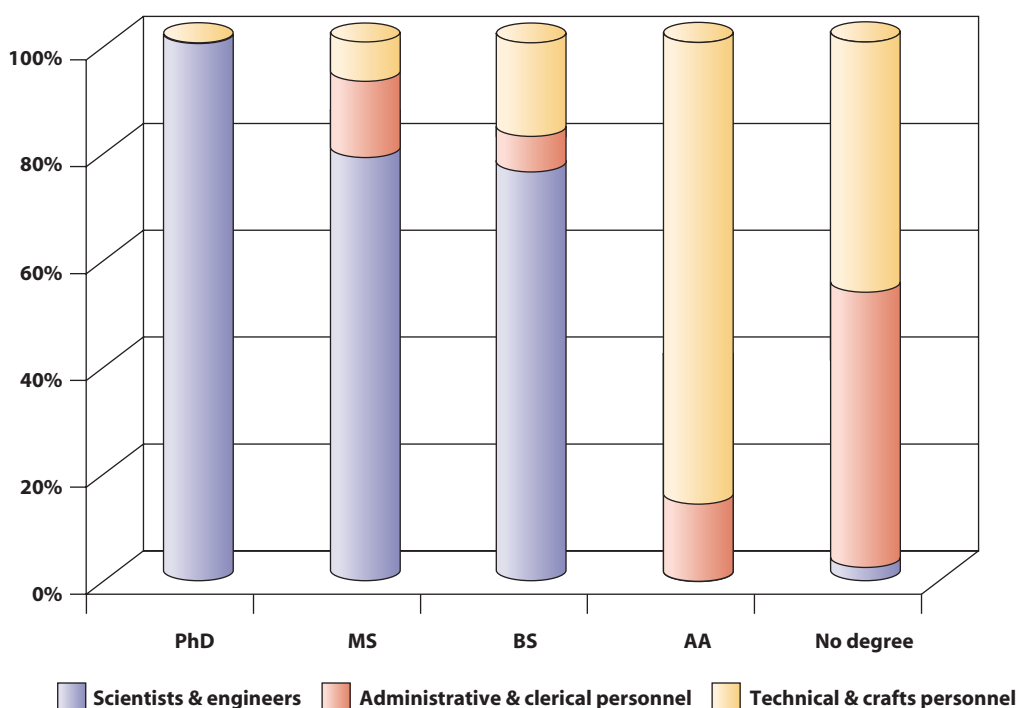


Table 8. CMS Staff Profile by Job Title and Degree Composition.

Job Title	PhD	MS	BS	AA	No degree	Total	Staff (%)
Scientists & Engineers	180	28	48	—	2	258	70
Physicist—(270)	47	2	—	—	—	49	13
Chemist—(242)	86	14	28	—	2	130	35
Engineer/Patent Engineer—(168, 249)	23	8	14	—	—	45	12
Mathematician/Computer Scientist—(256, 285)	—	—	1	—	—	1	—
Biological Scientist—(225, 277, 235, 228, 221)	—	—	3	—	—	3	1
Environmental Scientist—(230)	—	—	—	—	—	—	—
Metallurgist—(265)	24	4	2	—	—	30	8
Administrative & Clerical Personnel	—	5	4	4	34	47	13
Management—(196, 197)	—	3	—	—	—	3	1
Administrative—(100–162)	—	2	2	—	16	20	5
Clerical/General Services—(400–462)	—	—	2	4	18	24	7
Technical & Crafts Personnel	—	2	10	23	29	64	17
Technical—(302–339, 393, 347–391, 502–588, 593)	—	2	10	23	29	64	17
Total CMS Heads	180	35	62	27	65	369	100
Degree Composition (%)	49	9	17	7	18	100	

Includes career employees only
 Minor variances may occur due to rounding.
 Dated: September 30, 2002



The breakdown within the scientific and engineering disciplines is 17% physicists, 44% chemists, 15% engineers, 10% metallurgists, and 1% biological scientists (see Table 8). About 70% of the scientists and engineers in CMS have PhDs.

A breakdown of the scientific staff by discipline is shown, along with the number of postdoctoral researchers, in Table 9.

A staff profile by discipline spanning the past ten years is shown in Table 10.

Table 9. CMS Scientists and Engineers by Discipline and Postdoctoral Researchers.

Job Title	Total	Staff (%)
Scientists & Engineers	258	87
Physicist—(270)	49	17
Chemist—(242)	130	44
Engineer/Patent Engineer—(168, 249)	45	15
Mathematician/Computer Scientist—(256, 285)	1	—
Biological Scientist—(225, 277, 235, 228, 221)	3	1
Environmental Scientist—(230)	—	—
Metallurgist—(265)	30	10
Postdoctoral Researchers	38	13
Total CMS Heads	296	100
Includes career employees, term employees, and postdoctoral researchers only Dated: September 30, 2002		

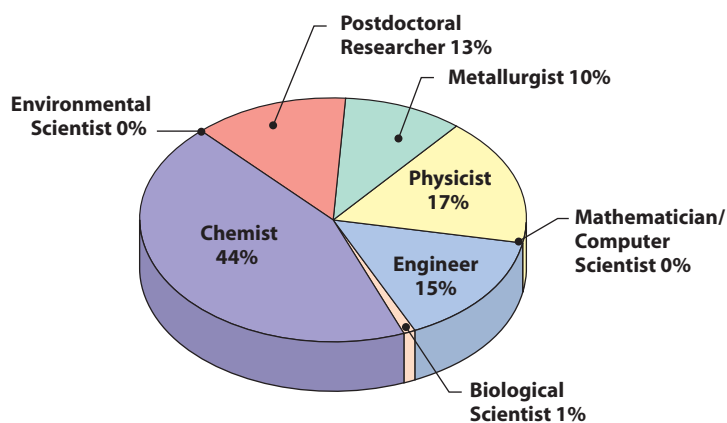
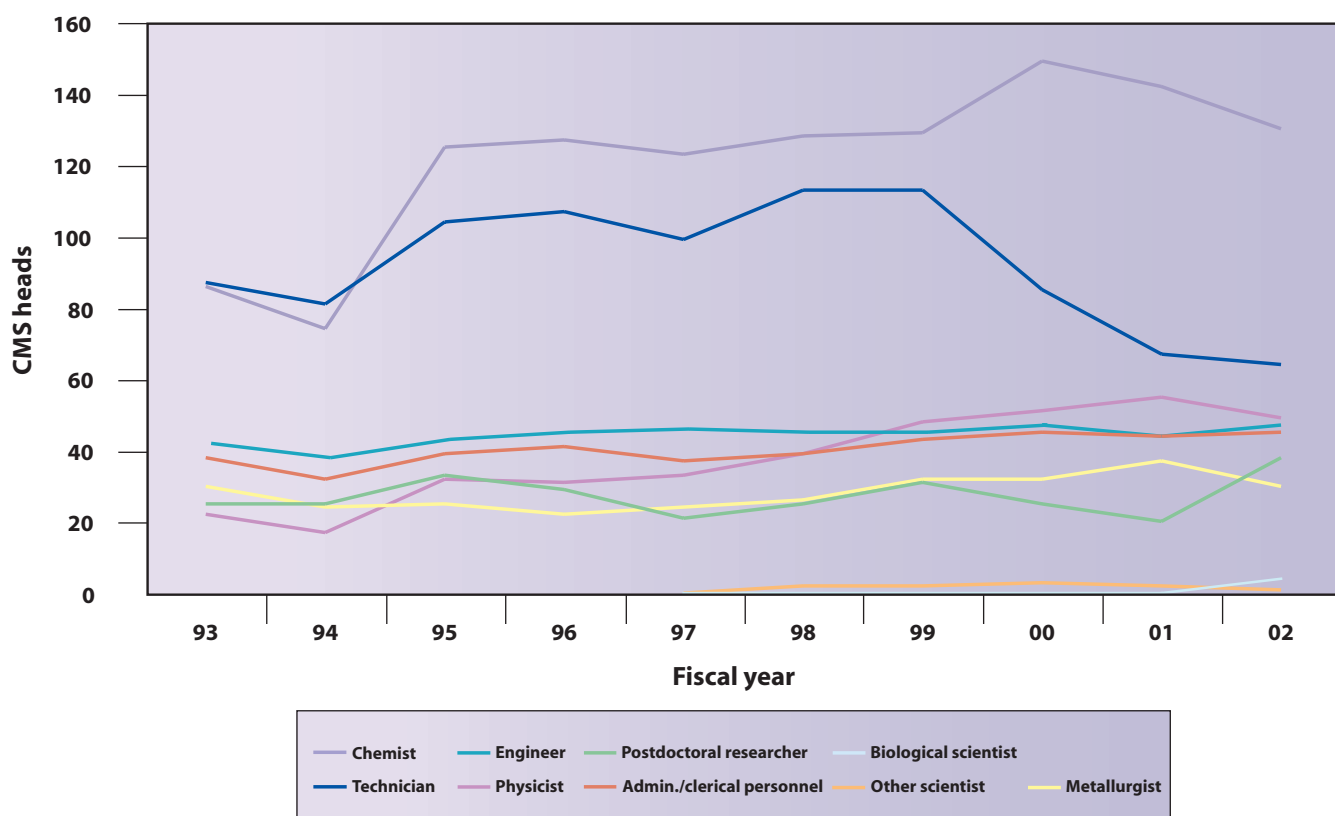


Table 10. Ten-Year CMS Staff Profile by Job Classification.

Discipline	1993	1994	1995	1996	1997	1998	1999	2000	2001	2002
Chemist	86	74	125	127	123	128	129	149	142	130
Physicist	22	17	32	31	33	39	48	51	55	49
Metallurgist	30	24	25	22	24	26	32	32	37	30
Engineer	42	38	43	45	46	45	45	47	44	45
Other Scientist	—	—	—	—	—	2	2	3	2	1
Biological Scientist	—	—	—	—	—	—	—	—	4	3
Postdoctoral Researcher	25	25	33	29	21	25	31	25	20	38
Technician	87	81	104	107	99	113	113	85	67	64
Admin./Clerical Personnel	38	32	39	41	37	39	43	45	44	47
Total CMS Heads	330	291	401	402	383	417	443	437	415	407
Excludes summer hires and supplemental laborers Dated: September 30, 2002										



Financial and Full-Time-Equivalent Highlights

Figure 6 illustrates how CMS will be funded in FY03 and is summarized as follows:

Internal CMS Funding

- Institutional Investment.** Funding comes from the Laboratory's general and administrative (G&A), institutional general-purpose equipment (IGPE), and Laboratory Directed R&D (LDRD) collections.
- CMS Infrastructure.** Funding comes from the CMS Directorate program management charge (PMC), organizational facility charge (OFC), and organizational personnel charge (OPC) collections.
- Discipline S&T.** Funding comes from DOE, federal, and non-federal sponsors.
- Program Support.** Funding comes from CMS Scientific Service Centers collections.

Non-CMS Funding

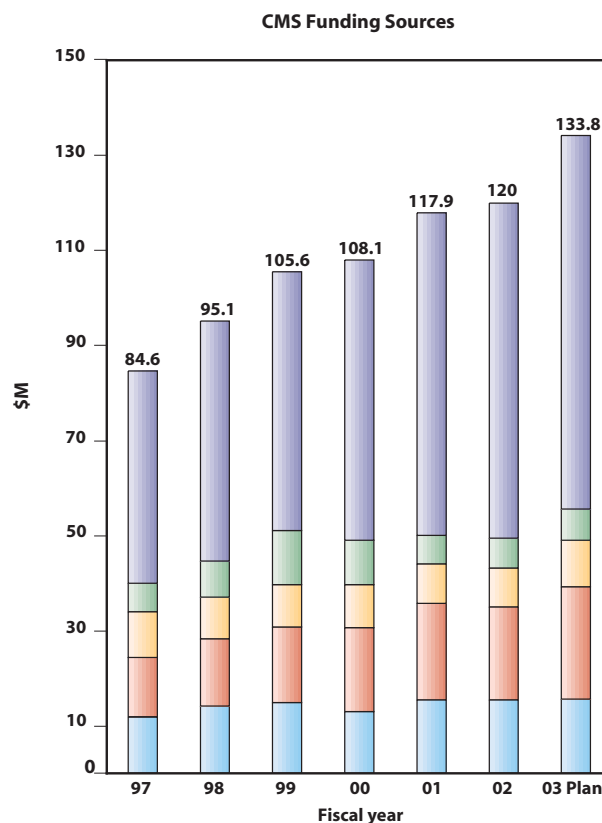
Program Support. The Directorate primarily provides discipline personnel for support to all Laboratory programs. Support for matrixed staff to program elements is received from other cost centers as FTE allocations.

Figure 6. How CMS Is Funded in FY03 (\$K).

CMS Funding Sources	
Total	133,816
Program Support	84,743
Discipline S&T	9,723
CMS Infrastructure	23,657
Institutional	15,693
Note: CMS-managed operating and capital totals \$55.7M.	

Program Support		Discipline S&T	
Program Support	84,743	Discipline S&T	9,723
297 CMS FTEs Matrixed		Office of Basic Energy Sciences (OBES)	2,806
(Other AD Cost Centers)	78,111	OBES Capital Equipment	421
Scientific Service Centers	6,632	Other DOE Direct	496
		Work for Others	6,000

CMS Infrastructure		Institutional Investment	
CMS Infrastructure	23,657	Institutional Investment	15,693
Facilities (OFC)	9,796	G&A	8,344
Information Systems (OFC)	2,074	Postdoctoral Fellows/Summer Hires	1,180
Personnel (OPC)	10,862	LDRD—Exploratory Research in the Disciplines	4,569
Program Management (PMC)	925	IGPE—Capital Equipment	1,600
		Note: The Deputy Director of S&T manages LDRD Lab-wide.	



Program support	44.5	50.4	54.5	59.0	67.8	70.5	78.1
Service centers	6.1	7.6	11.2	9.2	6.0	6.3	6.6
Discipline S&T	9.6	8.7	9.0	9.1	8.4	8.1	9.7
CMS infrastructure	12.6	14.2	15.8	17.7	20.2	19.6	23.7
Institutional investment	11.9	14.2	15.0	13.0	15.6	15.5	15.7

Distribution of FTEs and Funding

Table 11 shows a distribution of CMS FTEs for FY02 and as planned for FY03. CMS scientific services FTEs, along with the FTEs who are matrixed out to specific directorates, are shown to illustrate CMS support to Laboratory programs.

Table 11. Distribution of CMS FTEs.

	FY02	FY03 Plan
CMS Internal Programs	95	97
Discipline S&T	12	12
CMS Infrastructure	55	59
Institutional Investment	28	27
Program Support & Matrixed Out	306	327
Scientific Service Centers	25	30
DNT	122	129
NIF Inertial Confinement Fusion	45	42
E&E	29	30
NAI	39	47
PAT	5	5
BBRP	—	2
Engineering	4	4
SSEP	13	13
Various	24	26
Total CMS FTEs	401	424

Minor variances may occur due to rounding.

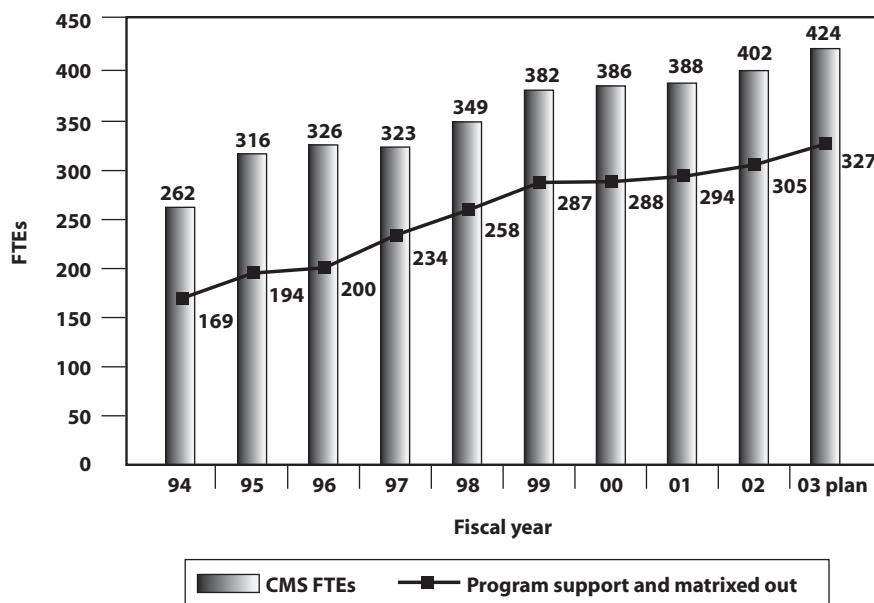


Table 12 shows how CMS-managed activities are supported according to funding sources. There are four categories:

- **Category 1: Discipline S&T** consists of research projects over which the directorate has jurisdiction. In FY02, this involved 12 FTEs of CMS personnel and 5 FTEs matrixed in from other organizations for a total budget of \$8.1M.
- **Category 2: CMS Infrastructure** consists of indirect activities involved in operating the Directorate. In FY02, this included 55 FTEs of CMS personnel and 37 FTEs matrixed in from other organizations for a total budget of \$19.6M.
- **Category 3: Institutional Investment** consists of indirect activities. In FY02, this included 28 FTEs of CMS personnel and 11 FTEs matrixed in from other organizations for a total budget of \$15.5M.
- **Category 4: Program Support** consists of scientific services (e.g., analytical and processing activities) supporting Laboratory programs. In FY02, this included 25 FTEs of CMS personnel and 6 FTEs matrixed in from other organizations for a total budget of \$6.3M.

Table 12. Distribution of Operating and Capital Funds (\$M) and FTEs for CMS Cost Centers.

	FY02 Actual 9/30/02			FY03 Planned as of 01/31/03		
	\$M	CMS FTEs	Other FTEs	\$M	CMS FTEs	Other FTEs
Category 1: Discipline S&T	8.1	12	5	9.7	12	2
DOE Direct	3.6	4	2	3.7	5	1
OBES (KC02)	2.9	3	2	2.8	4	1
OBES Capital Equipment/Fabrication	0.4	—	—	0.4	—	—
Other DOE Direct	0.3	—	—	0.5	1	—
Work for Others	4.5	8	3	6.0	8	1
Work for DOE	3.9	7	2	2.0	7	1
Federal Agencies	0.1	—	—	3.6	—	—
Non-Federal	0.6	1	—	0.4	—	—
Category 2: CMS Infrastructure	19.6	55	37	23.7	59	37
Organizational Personnel Charge	9.2	43	2	10.9	48	3
Program Management Charge	0.9	3	—	0.9	3	—
Organizational Facility Charge	9.5	8	35	11.9	7	34
Category 3: Institutional Investment	15.5	28	11	15.7	27	12
General & Administrative (G&A)	8.2	17	7	8.3	15	10
G&A—Special Employee Program (Postdoctoral Researchers/Summer Hires)	1.0	—	—	1.2	—	—
Institutional General-Purpose Equipment	1.3	—	—	1.6	—	—
LDRD—Exploratory Research in the Disciplines	5.0	11	3	4.6	12	2
Category 4: Program Support	6.3	25	6	6.6	30	7
Scientific Service Centers	6.3	25	6	6.6	30	7
Total CMS Operating & Capital	49.5	120	59	55.7	127	58
Minor variances may occur due to rounding.						

In FY02, the sum for the CMS-managed operating cost centers was \$47.8M with 179 FTEs (120 from CMS and 59 matrixed in). When added to the estimated cost of personnel matrixed (281 FTEs) to support the programs, the Directorate's total operating cost was about \$118.3M with a capital-equipment budget of \$1.7M, for a total of \$120M.

In FY03, the CMS-managed operating cost center is expected to be \$53.7M with

185 FTEs (127 from CMS and 58 matrixed in). When added to the estimated cost of personnel matrixed (297 FTEs) to support the programs, the Directorate's total operating cost would be about \$131.8M with a capital-equipment budget of \$2.0M, for a total of \$133.8M.

Figures 7 and 8 show operating and capital costs along with FTEs from FY94 to FY03 (planned).

Figure 7. Ten-Year Distribution of Operating and Capital Funds (\$M) for CMS Cost Centers.

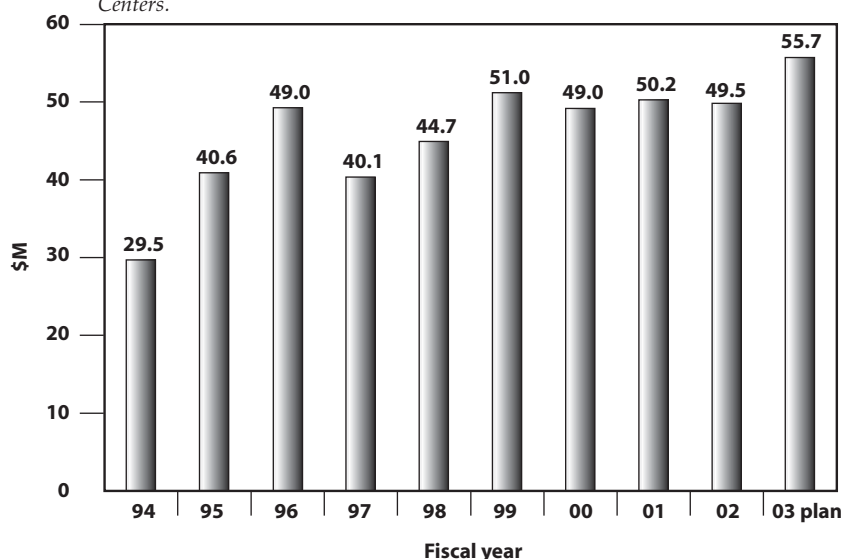
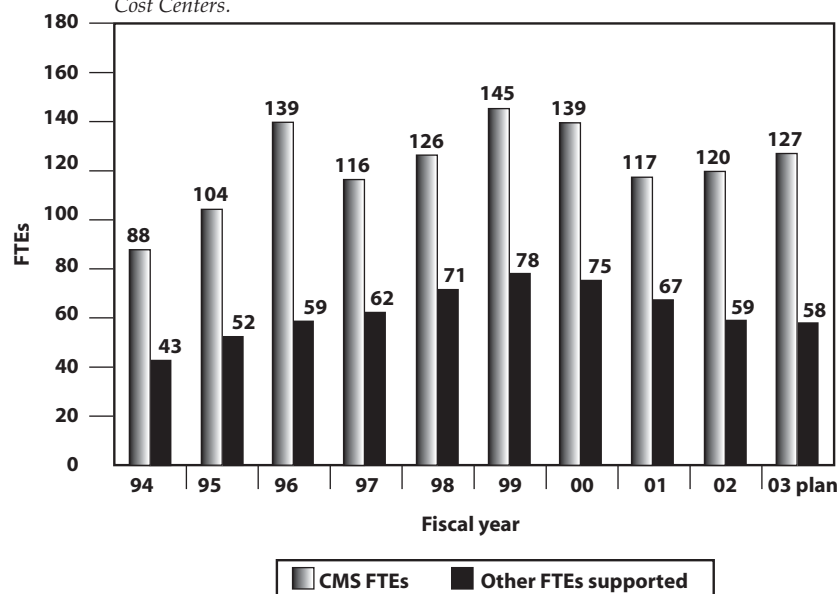


Figure 8. Ten-Year Distribution of CMS FTEs and Other FTEs Supported by CMS Cost Centers.



CMS Facilities at Site 200

Site 200, the Lawrence Livermore main site, is located within the Livermore city limits on one square mile of land. CMS facilities are in the heart of the Laboratory, and all CMS facilities are within walking distance (about five minutes) of one another.

CMS has several unique chemistry facilities needed to accomplish LLNL programmatic missions. These capabilities include isotope sciences and radiochemistry diagnostics; analytical and characterization services and technology; and material and chemical process theory, modeling, and computations.

Facilities Profile

The Directorate operates four facility complexes at Site 200: Buildings 132N, 151, 235, and 241 (see Table 13).

Table 13. CMS Site 200 Facilities Profile.

Building	Building Characteristics	Primary Functions	Facility Acquisition Cost
B132N/133: Chemistry Laboratories	<ul style="list-style-type: none"> • B132N—8 years old • B133—9 years old • 210,000 gross square feet • Limited access • Wet chemistry • 32 laboratories • 80 offices 	<ul style="list-style-type: none"> • Synthesis, formulation, and processing chemistry • Chemical analysis • Forensic science 	<ul style="list-style-type: none"> • Facility—\$34M • Equipment—\$12M
B151/154: Analytical and Isotopic Laboratories	<ul style="list-style-type: none"> • B151—35 years old • B154—12 years old • 111,000 gross square feet • Limited/controlled access • Wet chemistry • 71 laboratories • 123 offices 	<ul style="list-style-type: none"> • Isotope sciences and radiochemistry diagnostics • Analytical and characterization services and technology • Geochemistry • Stockpile stewardship • Glenn T. Seaborg Institute 	<ul style="list-style-type: none"> • Facility—\$49M • Equipment—\$15M
B235: Materials Science Laboratories	<ul style="list-style-type: none"> • 16 years old • 91,000 gross square feet • Limited/controlled access • Instrument laboratories • 30 laboratories • 116 offices 	<ul style="list-style-type: none"> • Materials development and technology • Material and chemical process theory, modeling, and computation • Materials characterization services and technology 	<ul style="list-style-type: none"> • Facility—\$29M • Equipment—\$29M
B241: Materials Technologies Facility	<ul style="list-style-type: none"> • 43 years old • 65,000 gross square feet • Controlled access • Instrument laboratories • 30 laboratories • 1 hi-bay • 40 offices 	<ul style="list-style-type: none"> • Materials development and technology • Materials disposition • Materials containment 	<ul style="list-style-type: none"> • Facility—\$21M • Equipment—\$7M

Organizational Facility Charge Collections

In FY02, OFC collections totaled \$9,492K (see Table 14).

OFC distributes the operations and maintenance costs of individual facilities owned by CMS. Distributing facility-related costs to residents of CMS facilities provides residents with an incentive for the efficient use and management of space.

CMS manages over 400,000 gross square feet of space. Types of space include laboratories, offices, cubicles, shops, and storage (e.g., cages and transportainers).

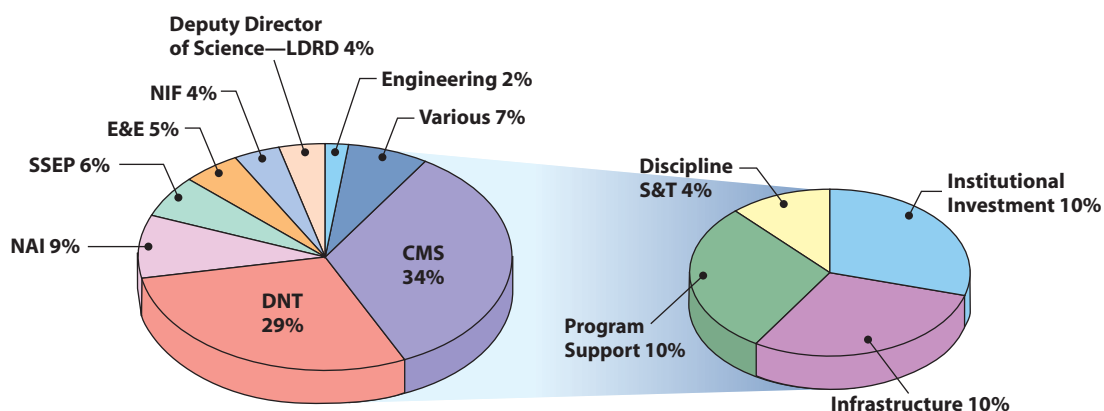
Operation and maintenance costs include the costs for facility management, facility coordinators, assurance oversight, information systems, property management, facility maintenance, and utilities and services (e.g., electricity, vehicles, copiers, telephones, and the laboratory facility charge).

Our information systems team provides support to more than 1,000 desktop computer systems in areas such as hardware and software installation, trouble resolution, and system administration. Other areas of responsibility include computer security, server administration, network installation, and connectivity.

Table 14. CMS Site 200 Space—Who Pays.

Directorate	FY02 (\$K)	%
CMS		
Program Support	997	10
Infrastructure	984	10
Institutional Investment	978	10
Discipline S&T	348	4
DNT	2,762	29
NAI	810	9
SSEP	581	6
E&E	486	5
NIF	371	4
Deputy Director of Science—LDRD	341	4
Engineering	174	2
Various	658	7
Total CMS Space	9,492	100

Minor variances may occur due to rounding.
Dated: September 30, 2002



CMS Facilities at Site 300

Site 300 is set on 7,000 acres of land about 15 miles east of Livermore. It is marked by both rolling hills and steep ravines, with very few trees in sight. When Site 300 was established in 1955, it was in a very remote area surrounded only by cattle ranches. Site 300 is still remote, but today the growing city of Tracy is expanding toward the site from the east.

At Site 300, CMS facilities are divided into three groups, as shown in Table 15: the chemistry area, the process area, and the Explosives Waste Storage Facility (EWSF) and the Explosives Waste Treatment Facility (EWTF).

Chemistry Area

The chemistry area is used to formulate and synthesize explosives compounds, scale up laboratory- and/or bench-scale size explosives formulations to production scale, and perform precision loading of shaped charges using extrusion technology.

Process Area

The process area is used to produce precision explosives parts and assemblies. The area facilities contain the machine tools, isostatic presses, radiography equipment, and precision assembly bays necessary for the manufacture of explosives parts.

Explosives Waste Storage Facility and Explosives Waste Treatment Facility

Explosives wastes are generated as a result of operations at Site 300 and the High Explosives Application Facility. The explosives waste facilities at Site 300 are EWSF and EWTF. Both facilities have California Department of Toxic Substances Control permits for the storage and treatment of explosives waste. EWSF is located in the process area and is used to store explosives waste for up to one year. EWTF is located at Building 845 in a remote area and is used for the open burning or detonation of explosives waste.

Table 15. CMS Site 300 Facilities Profile.

Facility	Facility Characteristics	Primary Functions	Capability
Chemistry Area *	<ul style="list-style-type: none"> • Between 34–43 years old • 8 formulations/synthesis/injection/molding • 2 mechanical pressing bays • 3 storage magazines 	<ul style="list-style-type: none"> • Synthesis • Formulation • Mechanical pressing • Scaleup 	<ul style="list-style-type: none"> • Custom manufacturing of explosives, with some transferred to industry for commercialization (e.g., simulants, special operations, shaped charges)
Process Area *	<ul style="list-style-type: none"> • Between 20–45 years old • 6 machine bays • 1 inspection bay • 4 assembly bays • 1 radiography bay • 1 isostatic pressing bay • 1 explosives heating bay • 2 surface impoundments 	<ul style="list-style-type: none"> • Hot isostatic press • Radiography • Machining • Inspection • Assembly 	<ul style="list-style-type: none"> • Precision, custom manufacturing of explosives components and devices for R&D testing
Explosives Waste	<ul style="list-style-type: none"> • Between 6–49 years old • Former storage magazines and shot test facility • 5 storage magazines • 1 control bunker • 1 detonation pad • 1 burn cage • 1 burn pan 	<ul style="list-style-type: none"> • Storage • Treatment 	<ul style="list-style-type: none"> • State-permitted storage facility for 1 year of storage • State-permitted treatment facility with open-burn/open-detonation capabilities
<p>* The chemistry and process areas comprise 22 major facilities, 14 storage magazines, and 8 service magazines for a total of 58,500 square feet and an equipment replacement cost of \$30M.</p>			

Research Administration and Funding

Research is considered an integral part of the Directorate's discipline development. Oversight and policy-making are vested in the AD's office. Currently, the Deputy AD for S&T assumes general responsibility for administering the research effort, with guidance from the CMS AD and consultation with Division and Program Leaders. Programs and projects are reviewed internally as well as externally. Funding for R&D that is managed in the Directorate comes primarily from LDRD, the DOE Office of Basic Energy Sciences (DOE/OBES), and reimbursable work for others.

Laboratory Directed Research and Development

An order issued by DOE provides for an LDRD program that uses an annual percentage (6% for FY02) of the Laboratory's budget for discretionary research. Livermore's LDRD program is divided into three major funding categories: Strategic Initiatives (SIs); Exploratory Research in the Disciplines (ERD), Programs, and Institutes; and Laboratory-Wide Competition (LW).

Strategic Initiatives

SI projects must be strongly aligned with the Laboratory's strategic directions and long-term vision. An SI project should describe innovative R&D activities that are likely to set new directions for existing programs, that will help develop new programmatic areas within our mission responsibilities, and/or that will enhance the Laboratory's S&T base. In the realm of SIs, CMS scientists may either lead SIs as principal investigators or participate as key team members on program-sponsored initiatives.

Exploratory Research in the Disciplines, Programs, and Institutes

These R&D activities are intended to support pioneering R&D projects that set new directions for the Laboratory and/or enhance the core competencies and the S&T base for the Laboratory. ERD is funded by R&D collections returned to the directorates that generate the funds. Such funds are designated to provide the technical base for developing both existing and future programs for the Laboratory. CMS frequently plays a role in these projects, through personnel supporting the execution of the science and occasionally by providing the leader for the project. In general, support for a project is limited to, at most, three consecutive years in this program. Table 16 shows FY03 CMS ERD projects.

The primary focus of CMS within its LDRD ERD portfolio is to support the longer-range research objectives of the Laboratory's programs. CMS influences the direction and development of these objectives by contributing to new science and capabilities. Two strategic objectives define how CMS uses its ERD portfolio:

1. **Program-Related ERDs.** Fundamental research that provides a basic scientific understanding of a specific issue faced by a program and acknowledged by the program as being important. CMS refers to this as program-related LDRD, and in many cases, CMS is successful in encouraging programs to coinvest their LDRD funds on these projects. Table 16 summarizes program-related CMS projects and associated programmatic coinvestments.
2. **New Scientific Capabilities.** Development of new science and capabilities focused on chemistry that will seed enduring, externally funded, fundamental science in areas of current or future importance to the Laboratory. CMS refers to this grouping of projects as new scientific capabilities. In some cases, these projects represent a new focus area such as computational chemistry, biochemistry, health sciences, and nanosciences, as shown in Table 16.

Table 16. CMS FY03 LDRD Projects and Funding.

CMS Contact	Project Title	Funding (\$K)	Directorate Cofunded (\$K)
Exploratory Research in the Disciplines (ERD)			
Program-Related ERD—DNT			
Allen	01-ERD Thermodynamics and Structure of Plutonium Alloys	144	326
Campbell	01-ERD Shear Localization and Fracture in Shocked Metals	90	153
King	03-ERD Determination of the Microstructural Morphology of Shock-Induced Melt and Resolidification	192	—
McNaney	03-ERD Preparation for Ultrahigh Pressure	144	50
Schwartz	01-ERD Metastability and Delta-Phase Retention in Plutonium Alloys	173	326
Wong	03-ERD Phono Dispersion Curves Determination in Delta-Phase Pu–Ga Alloys	120	289
Program-Related ERD—NAI			
Gard	02-ERD Single Cell Proteomics with Ultrahigh-Sensitivity Mass Spectrometry	288	235
Moody	02-ERD Investigation of the Shores of the Island of Stability	240	—
Reynolds	01-ERD Nanoscience and Nanotechnology in Nonproliferation Applications	96	200
Westbrook	02-ERD Atmospheric Reactive Flow Modeling and Experiments	125	140
Wilson	03-ERD Spider	363	—
Program-Related ERD—E&E			
Denison	03-ERD Resolving Nuclear Reactor Lifetime Extension	144	120
Moran	03-ERD Transport and Biogeochemical Cycling of Iodine-129 from Nuclear Fuel Reprocessing Facilities	163	—
New Scientific Capabilities—Computational Chemistry			
A. Quong	02-ERD A 3-D Model of Signaling and Transport Pathways in Epithelial Cells	216	—
New Scientific Capabilities—Biochemistry/Health Services			
De Yoreo	01-ERD Dip-Pen Nanolithography for Controlled Deposition of Proteins and Colloids	407	—
Hollars	02-ERD Development of Ultrasensitive High-Speed Biological Assays Based on 2-D Flow Cell Detection of Single Molecules	201	261
Letant	03-ERD DNA Detections through Designed Apertures	250	30
Perkins	01-ERD Development of Synthetic Antibodies	240	115
J. Quong	01-ERD Imaging of Isotopically Enhanced Molecular Targeting Agents	240	75
New Scientific Capabilities—Nanoscience			
Eaglesham	03-ERD Carbon-Nanotube Permeable Membranes	400	—
Nieh	01-ERD Enhancement of Strength and Ductility in Bulk Nanocrystalline Metals	163	—
New Scientific Capabilities—General			
Bakajin	02-ERD Development of a Fast Microfluidic Mixer for Studies of Fast Protein Folding Kinetics	75	—
Total ERD		4,469	2,320
Laboratory-Wide Competition (LW)			
Cai	03-LW Long-Time-Scale Atomistic Simulations	—	145
Glaesemann	02-LW Quantum Vibrations in Molecules	—	149
Hart	03-LW Laser-Initiated Nanoscale Molecularly Imprinted	—	185
Hope-Weeks	03-LW Covalent Attachment of Metallic Nanorods	—	100
Huser	03-LW Coherent Anti-Stokes Raman Microscopy	—	150
Shields	02-LW Photoluminescent Silica Sol-Gel	—	186
Total LW		—	916

Minor variances may occur due to rounding.

CMS's selection process focuses on projects meeting these strategic objectives, but it also considers several other important criteria:

- Projects must be based on the execution of excellent science.
- Whenever possible, projects should provide an opportunity for more experienced scientists in CMS to work with younger staff—and especially postdoctoral researchers—in a mentoring relationship.
- Partnering and collaboration with other Directorates is encouraged in all areas and is required for program-related research.

Laboratory-Wide Competition

Projects in this category emphasize innovative research concepts and ideas with limited management filtering to encourage the creativity of individual researchers. Table 16 also includes six projects funded from LW, which is managed by the Laboratory's S&T Deputy Director.

DOE Direct

The Directorate coordinates funds obtained from the Office of Basic Energy Sciences (OBES) Division of Materials Sciences (DMS), which total \$2.8M for FY03 (see Table 17). CMS is responsible for executing the majority of the program, as well as for reporting, oversight, and review of the entire program. The Livermore OBES/DMS program has three major components:

- The **Metallurgy and Ceramics Program** addresses a diverse range of topics, including adhesion and bonding at internal interfaces, fundamental characterization and modeling of welding processes, as well as research focused on the fundamentals of superplastic deformation.
- The **Solid-State Physics Program** has three components addressing new concepts in modeling radiation damage in solids; the development and characterization of new optical materials, including new lasing materials; and the development of positron science as a key materials characterization technique.

Table 17. CMS FY03 OBES Projects and Budgets.

CMS Contact	Project Title	Operating (\$K)	Capital (\$K)
Materials Science			
Baumann	Nanoscience Polymers	48	—
Bulatov	Microstructural Effects on Mechanics of Materials	50	—
Campbell/King	Adhesion & Bonding at Internal Interfaces Studies	280	—
Elmer/Wong	Welding Metallurgy Group	492	—
Nieh	Interfaces & Interphases on Superplasticity	176	—
A. Quong	Physical Properties	60	—
A. Quong	Radiation Damage	186	—
Terminello	Capital Equipment—TBD	—	421
Terminello	Center of Excellence Synthesis Processing	85	—
Terminello	Growth & Formation of Advanced Heterointerfaces	375	—
Tobin	Investigation of Nanoscale Magnetism	358	—
Total CMS OBES		2,110	421
Other			
Asoka-Kumar/Dension	PAT—Positron Research	380	—
Payne	LS&T Optical Materials	209	—
Terminello	PAT KC0206 Funding—TBD	107	—
Total Other OBES		696	—
Grand Total OBES		2,806	421

- The **Materials Chemistry Program** addresses the science of thin, buried layers and the exploration of innovative new techniques for characterizing magnetic properties at the atomic level.

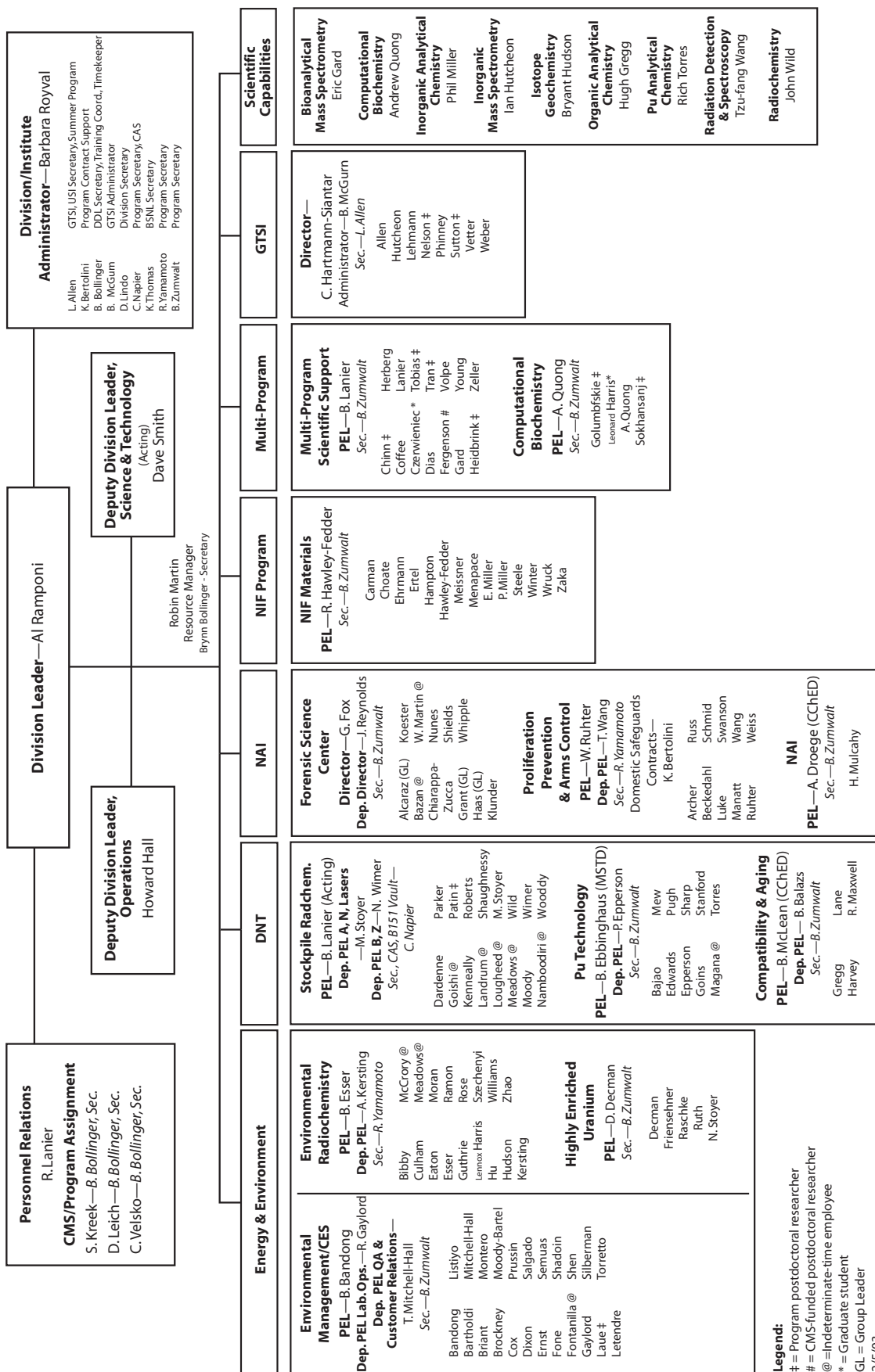
Scientific and Technical Achievements

Table 18 lists some of the Directorate's scientific and technical achievements for the 2002 calendar year.

Table 18. CMS Scientific and Technical Achievements in 2002.

Metric	2002
Major Awards	2
R&D 100 Awards	1
Patent Disclosures	30
Patent Applications	20
Patents Issued	17
Licenses Executed	5
Refereed Publications	260
Invited Presentations (Major Conferences)	75
Contributed Presentations	200
Journal Editorships	6
Conferences Organized	8
Editorial Boards	6

Analytical and Nuclear Chemistry Division


Legend:

= Program postdoctoral researcher
 # = CMS-funded postdoctoral researcher
 @ = Indeterminate-time employee
 * = Graduate student
 GL = Group Leader
 2/5/03

Chemistry and Chemical Engineering Division

